Support Vector Machines

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July 21, 2025

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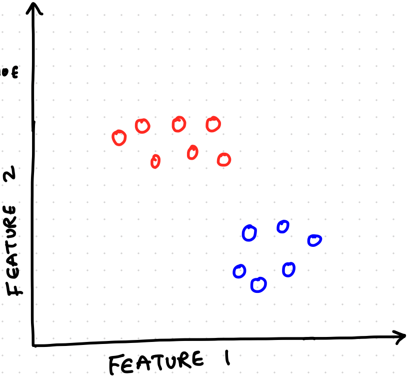
Outline

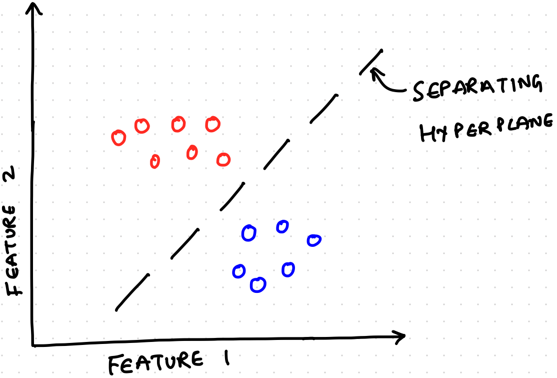
Introduction and Motivation

SUPPORT VECTOR MACHINES

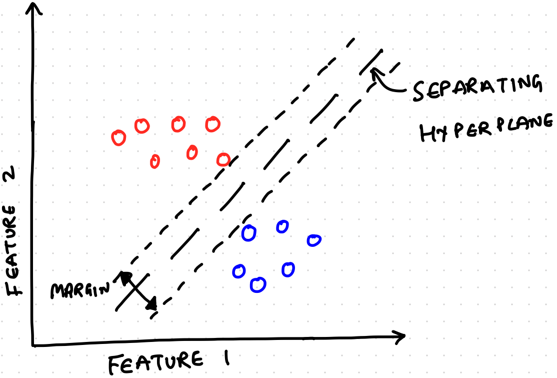
POPULAR BINARY

CLASSIFICATION TECHNIQUE

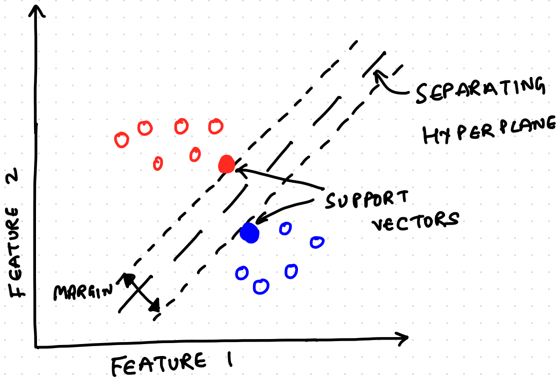




IDEA: DRAW A SEPARATING HYPERPLANE



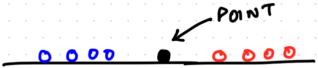
IDEA: MAXIMIZE THE MARGIN



SUPPORT VECTORS: POINTS ON BOUNDARY | MARGIN

HYPERPLANE V/S # DIMENSIONS

1D



HYPERPLANE V/S # DIMENSIONS

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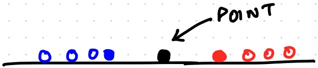
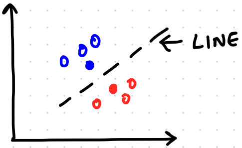


2D



HYPERPLANE V/S # DIMENSIONS

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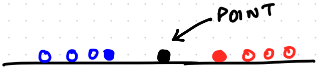
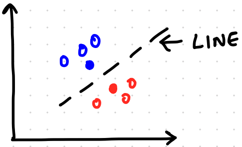
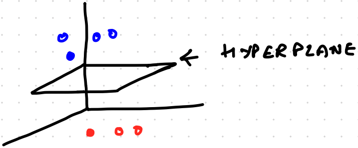


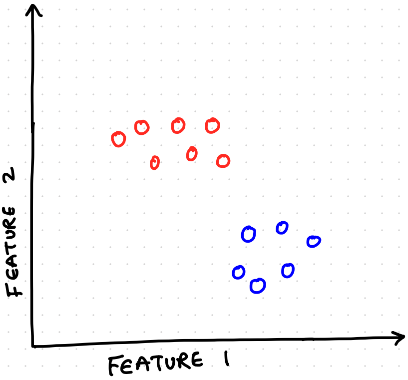
2D



3D
(AND
MORE)



WHICH HYPERPLANE?



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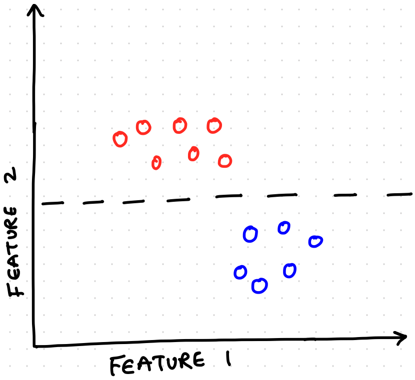

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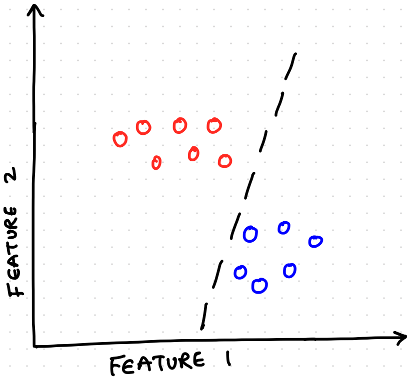

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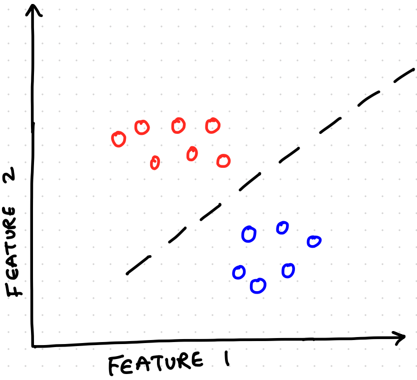
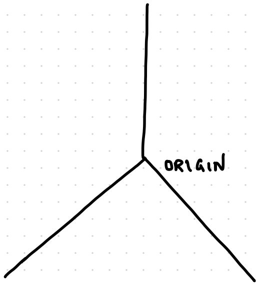
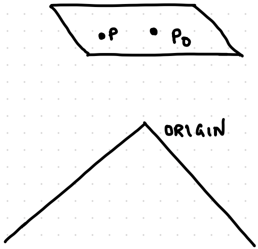


EQUATION OF HYPERPLANE

HOW TO DEFINE?



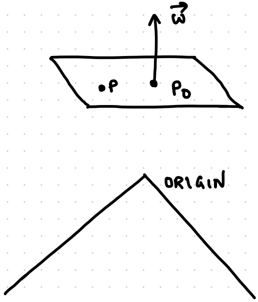
EQUATION OF HYPERPLANE



P: Any point on plane

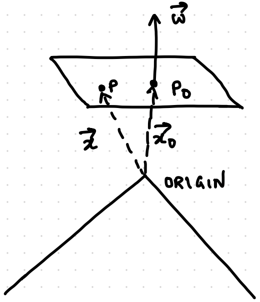
P_0: One point on plane

EQUATION OF HYPERPLANE



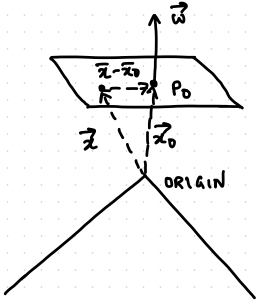
$\vec{w}$: $\perp$ vector to plane at P_0

EQUATION OF HYPERPLANE



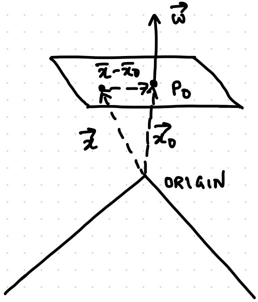
P and P_0 lie on plane

EQUATION OF HYPERPLANE



$\overrightarrow{P P_0} = \vec{x} - \vec{x}_0$ lies on plane

EQUATION OF HYPERPLANE



$\overrightarrow{P P_0} = \vec{x} - \vec{x}_0$ lies on plane

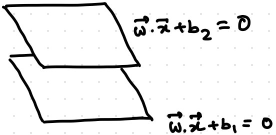
$\Rightarrow \vec{w} \perp (\vec{x} - \vec{x}_0)$

or, $\vec{w} \cdot (\vec{x} - \vec{x}_0) = 0$

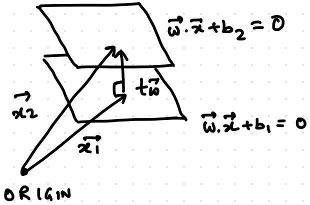
or, $\vec{w} \cdot \vec{x} - \vec{w} \cdot \vec{x}_0 = 0$

or, $\boxed{\vec{w} \cdot \vec{x} + b = 0}$

DISTANCE B/W ∥ HYPERPLANES



DISTANCE B/W || HYPERPLANES



Mathematical Foundation

Distance between 2 parallel hyperplanes

Equation of two planes is:

$$\mathbf{w} \cdot \mathbf{x} + b_1 = 0$$

$$\mathbf{w} \cdot \mathbf{x} + b_2 = 0$$

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For a point $\mathbf{x}_1$ on plane 1 and $\mathbf{x}_2$ on plane 2, we have:

$$\mathbf{x}_2 = \mathbf{x}_1 + t\mathbf{w}$$
$$D = |t\mathbf{w}| = |t|\|\mathbf{w}\|$$

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We can rewrite as follows:

$$\mathbf{w} \cdot \mathbf{x}_2 + b_2 = 0$$
$$\Rightarrow \mathbf{w} \cdot (\mathbf{x}_1 + t\mathbf{w}) + b_2 = 0$$

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We can rewrite as follows:

$$\mathbf{w} \cdot \mathbf{x}_2 + b_2 = 0$$
$$\Rightarrow \mathbf{w} \cdot (\mathbf{x}_1 + t\mathbf{w}) + b_2 = 0$$

$$\Rightarrow \mathbf{w} \cdot \mathbf{x}_1 + t\|\mathbf{w}\|^2 + b_1 - b_1 + b_2 = 0 \Rightarrow t = \frac{b_1 - b_2}{\|\mathbf{w}\|^2} \Rightarrow D = t\|\mathbf{w}\| = \frac{|b_1 - b}{\|\mathbf{w}\|}$$

Pop Quiz #1

Quick Question!

If two parallel hyperplanes are given by:

- $\mathbf{w} \cdot \mathbf{x} + 3 = 0$

And $\|\mathbf{w}\| = 2$, what is the distance between them?

Pop Quiz #1

Quick Question!

If two parallel hyperplanes are given by:

- $\mathbf{w} \cdot \mathbf{x} + 3 = 0$
- $\mathbf{w} \cdot \mathbf{x} - 1 = 0$

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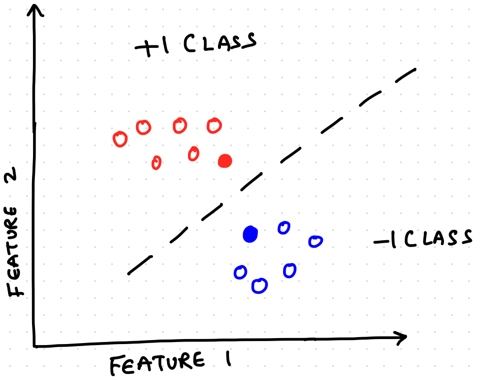
- $\mathbf{w} \cdot \mathbf{x} + 3 = 0$
- $\mathbf{w} \cdot \mathbf{x} - 1 = 0$

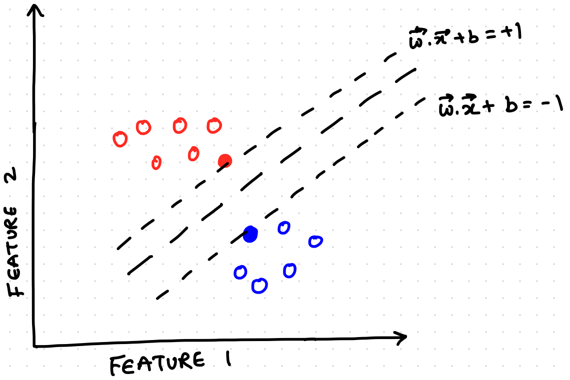
And $\|\mathbf{w}\| = 2$, what is the distance between them?
Answer: $D = \frac{|3-(-1)|}{2} = \frac{4}{2} = 2$ units

SVM Formulation

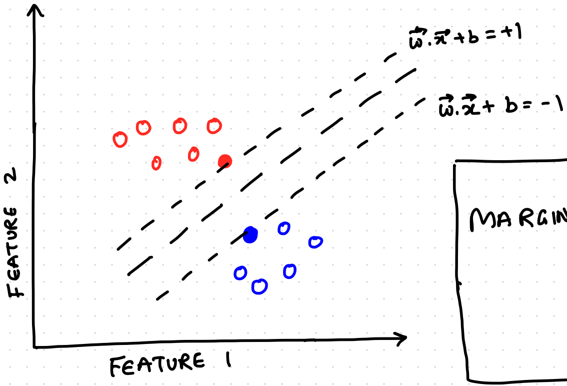
FORMULATION



FORMULATION

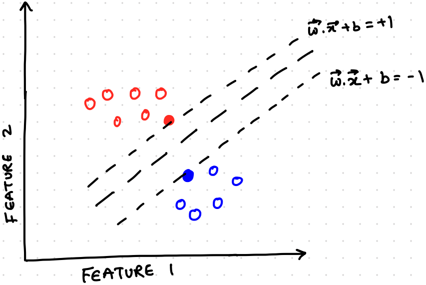


FORMULATION



$$\text{MARGIN} = \frac{(b+1)-(b-1)}{\|\vec{w}\|} = \frac{2}{\|\vec{w}\|}$$

FORMULATION



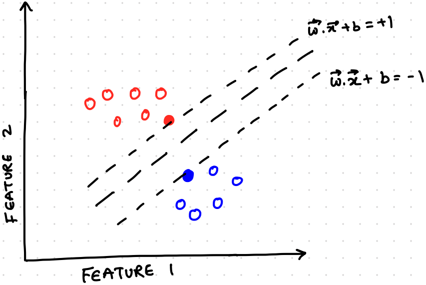
GOAL: MAXIMIZE MARGIN

$\Rightarrow$ MAXIMIZE $\dfrac{2}{||\vec{w}||}$

$\Rightarrow$ MINIMIZE $||\vec{w}||$

S.T. Correctly label points

FORMULATION



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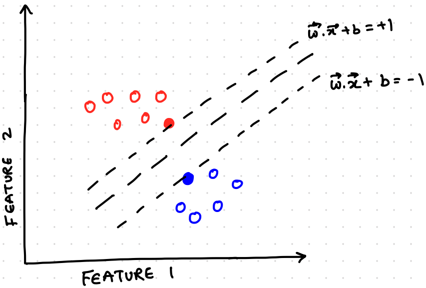
i.e. if $y_i = -1$

$\vec{w}.\vec{x}+b \leq -1$

if $y_i = +1$

$\vec{w}.\vec{x}+b \geq 1$

FORMULATION



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if $y_i = +1$

$\vec{w}.\vec{x}+b \geq 1$

$$\boxed{y_i\,(\vec{w}.\vec{x}+b) \geq 1}$$

Primal Formulation

Objective

$$\begin{aligned} &\text{minimize} \frac{1}{2}\|\mathbf{w}\|^2 \\ &\text{subject to} y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1 \quad \forall i \end{aligned}$$

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$$\text{minimize} \frac{1}{2}\|\mathbf{w}\|^2$$
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Q) What is $\|\mathbf{w}\|$?

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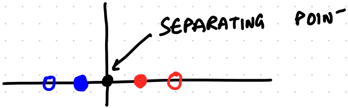
Q) What is $\|\mathbf{w}\|$?

$$\mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix}$$

$$\|\mathbf{w}\| = \sqrt{\mathbf{w}^\top \mathbf{w}}$$
$$= \sqrt{\begin{bmatrix} w_1 & w_2 & \cdots & w_n \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix}}$$

Worked Example

EXAMPLE (IN 1D)



$$\begin{bmatrix} x & y \\ 1 & 1 \\ 2 & 1 \\ -1 & -1 \\ -2 & -1 \end{bmatrix}$$

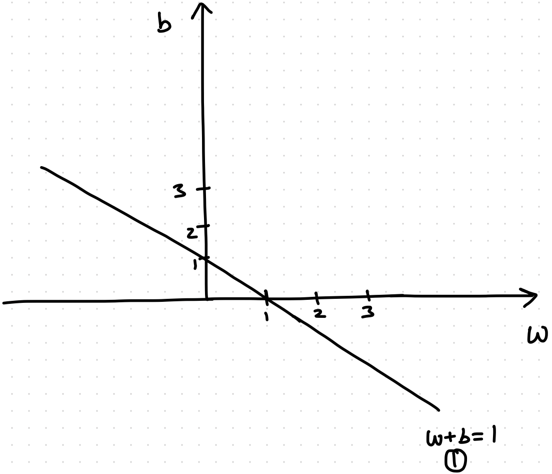
Separating Hyperplane: $\mathbf{w} \cdot \mathbf{x} + b = 0$

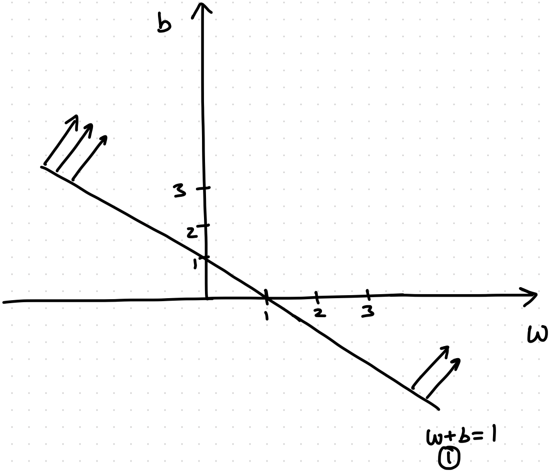
Simple Exercise

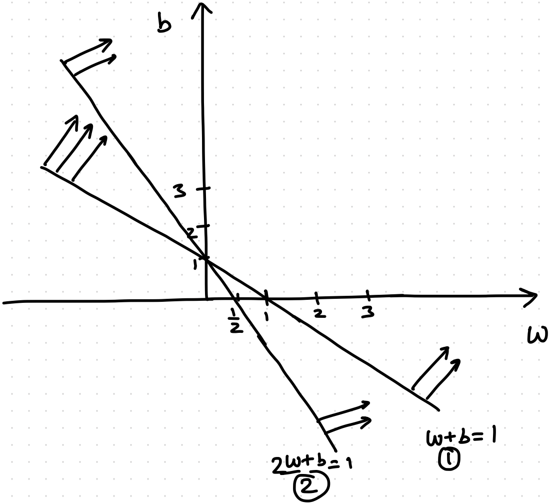
$$y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1$$

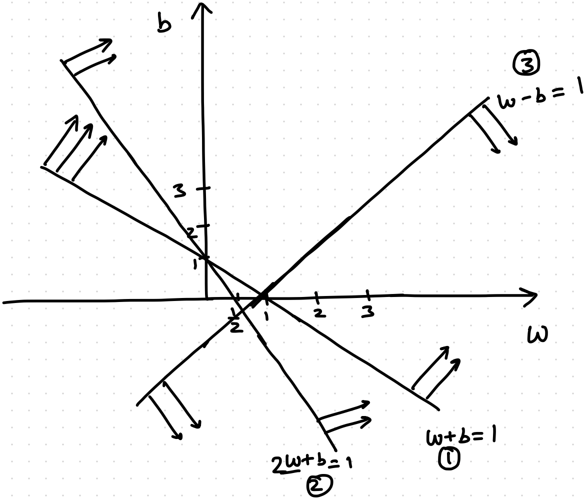
$$\begin{bmatrix} x_1 & y \\ 1 & 1 \\ 2 & 1 \\ -1 & -1 \\ -2 & -1 \end{bmatrix}$$

$$\begin{aligned}
&\Rightarrow y_i(w \cdot x_i + b) \geq 1 \\
&\Rightarrow 1(w \cdot 1 + b) \geq 1 \\
&\Rightarrow 1(w \cdot 2 + b) \geq 1 \\
&\Rightarrow -1(w \cdot (-1) + b) \geq 1 \\
&\Rightarrow -1(w \cdot (-2) + b) \geq 1
\end{aligned}$$

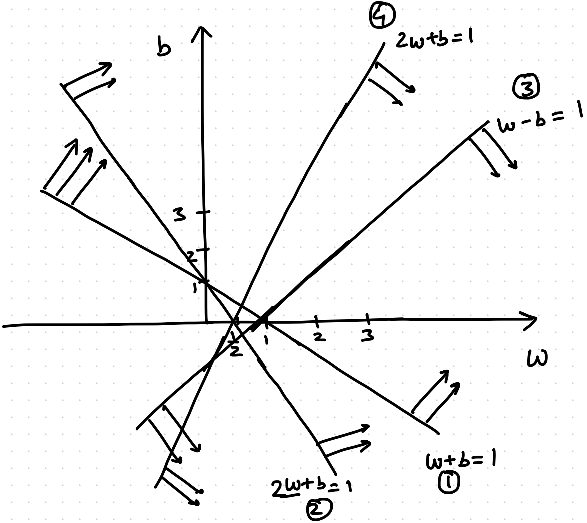

b
3
2
1
1
2
3
w
w+b=1
1


b
3
2
1
1
2
3
w
w+b=1
1

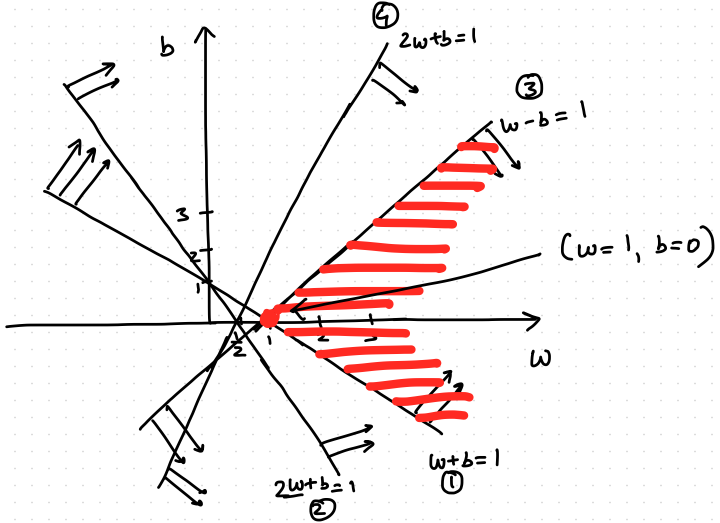

b
3
2
1
1/2
1
2
3
w
w+b=1
1
2w+b=1
2



b
w
3
2
1
1/2
1
2
3
③
w-b=1
w+b=1
①
2w+b=1
②



b
w
1
2
3
$\frac{1}{2}$
1
2
3
④ $2w+b=1$
③ $w-b=1$
$w+b=1$ ①
$2w+b=1$ ②



4
2w+b=1
3
w-b=1
b
3
2
1
(w=1, b=0)
1/2
1
2
3
w
w+b=1
1
2w+b=1
2

Simple Exercise

$$
\begin{aligned}
w_{min} &= 1, b = 0 \\
w.x + b &= 0 \\
x &= 0
\end{aligned}
$$

Simple Exercise

Minimum values satisfying constraints $\Rightarrow w = 1$ and $b = 0$

$\therefore$ Max margin classifier $\Rightarrow x = 0$

Pop Quiz #2

Think About This!

In our simple 1D example, why did we choose $w = 1$ and $b = 0$ as the optimal solution?

Pop Quiz #2

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- Is this the **only** solution that separates the data?

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In our simple 1D example, why did we choose $w = 1$ and $b = 0$ as the optimal solution?

- Is this the **only** solution that separates the data?
- What makes this solution **optimal** for SVM?

Answer: No, infinitely many solutions exist (e.g., $w = 2, b = 0$ or $w = 0.5, b = 0$).
SVM chooses $w = 1, b = 0$ because it minimizes $\|\mathbf{w}\|^2$ while satisfying all constraints!

Primal Formulation is a Quadratic Program

Generally;

$\Rightarrow$ Minimize Quadratic(x)

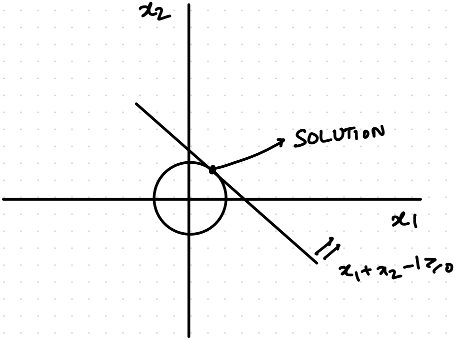
$\Rightarrow$ such that, Linear(x)

Question

$$x = (x_1, x_2)$$
$$\text{minimize} \quad \frac{1}{2}||x||^2$$
$$: x_1 + x_2 - 1 \geq 0$$

MINIMIZE QUADRATIC

S.t. LINEAR



Converting to Dual Problem

Primal $\Rightarrow$ Dual Conversion using Lagrangian multipliers

$$\text{Minimize } \frac{1}{2}\|\mathbf{w}\|^2$$
$$\text{s.t. } y_i(\mathbf{w}\cdot\mathbf{x}_i + b) \geq 1$$
$$\forall i$$

$$L(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\sum_{i=1}^{d} w_i^2 - \sum_{i=1}^{N}\alpha_i(y_i(\mathbf{w}\cdot\mathbf{x}_i + b) - 1) \ \forall \ \alpha_i \geq 0$$
$$\frac{\partial L}{\partial b} = 0 \Rightarrow \sum_{i=1}^{n}\alpha_i y_i = 0$$

Converting to Dual Problem

$$\frac{\partial L}{\partial \mathbf{w}} = 0 \Rightarrow \mathbf{w} - \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i = 0$$

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$$

$$L(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2} \sum_{i=1}^{d} w_i^2 - \sum_{i=1}^{N} \alpha_i (y_i (\mathbf{w} \cdot \mathbf{x}_i + b) - 1)$$

$$= \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^{N} \alpha_i y_i \mathbf{w} \cdot \mathbf{x}_i - \sum_{i=1}^{N} \alpha_i y_i b + \sum_{i=1}^{N} \alpha_i$$

$$= \sum_{i=1}^{N} \alpha_i + \frac{\left(\sum_i \alpha_i y_i \mathbf{x}_i\right) \cdot \left(\sum_j \alpha_j y_j \mathbf{x}_j\right)}{2} - \sum_i \alpha_i y_i \left(\sum_j \alpha_j y_j \mathbf{x}_j \right) \cdot \mathbf{x}_i$$

Converting to Dual Problem

$$L(\boldsymbol{\alpha}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j$$

Minimize $\|\mathbf{w}\|^2 \Rightarrow$	Maximize $L(\boldsymbol{\alpha})$
$s.t$	$s.t$
$y_i \left(\mathbf{w} \cdot \mathbf{x}_i + b \right) \geqslant 1$	$\sum_{i=1}^{N} \alpha_i y_i = 0 \ \forall \ \alpha_i \geq 0$

Pop Quiz #3

Lagrangian Mystery!

Why do we convert the primal SVM problem to its dual formulation?

Pop Quiz #3

Lagrangian Mystery!

Why do we convert the primal SVM problem to its dual formulation?

Hint: Think about what the dual formulation enables us to do that the primal doesn't...

Pop Quiz #3

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Answer: The dual formulation enables the **kernel trick**!

- Primal: $\mathbf{w}$ appears explicitly $\rightarrow$ no kernels

Pop Quiz #3

Lagrangian Mystery!

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Hint: Think about what the dual formulation enables us to do that the primal doesn't...

Answer: The dual formulation enables the **kernel trick**!

- Primal: $\mathbf{w}$ appears explicitly $\rightarrow$ no kernels
- Dual: Only dot products $\mathbf{x}_i \cdot \mathbf{x}_j$ appear $\rightarrow$ can replace with $K(\mathbf{x}_i, \mathbf{x}_j)$

Question: KKT Complementary Slackness

Question:

$\alpha_i \left(y_i \left(\mathbf{w} \cdot \mathbf{x}_i + b\right) - 1\right) = 0 \quad \forall i$ as per KKT slackness

What is α_i for support vector points?

Answer: For support vectors,

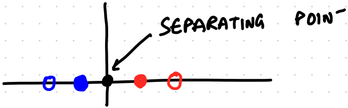
$$\mathbf{w} \cdot \mathbf{x}_i + b = -1 \text{ (for } y_i = -1)$$
$$\mathbf{w} \cdot \mathbf{x}_i + b = +1 \text{ (for } y_i = +1)$$

$y_i \left(\mathbf{w} \cdot \mathbf{x}_i + b\right) - 1 = 0 \quad$ for $i \in \{$support vector points$\}$

$\therefore \alpha_i \neq 0$ where $i \in \{$support vector points$\}$

For all non-support vector points: $\alpha_i = 0$

EXAMPLE (IN 1D)



Revisiting the Simple Example

$$\begin{bmatrix} x_1 & y \\ 1 & 1 \\ 2 & 1 \\ -1 & -1 \\ -2 & -1 \end{bmatrix}$$

$$L(\boldsymbol{\alpha}) = \sum_{i=1}^{4} \alpha_i - \frac{1}{2} \sum_{i=1}^{4} \sum_{j=1}^{4} \alpha_i \alpha_j y_i y_j x_i x_j \qquad \alpha_i \geq 0$$

$$\sum \alpha_i y_i = 0 \qquad \alpha_i(y_i(w \cdot x_i + b) - 1) = 0$$

Pop Quiz #4

Support Vector Challenge!

In our 1D example with data points $\{(1, +1), (2, +1), (-1, -1), (-2, -1)\}$, which points will be the support vectors?

Pop Quiz #4

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Think: Support vectors are the closest points to the decision boundary that actively constrain the solution.

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Think: Support vectors are the closest points to the decision boundary that actively constrain the solution.

Answer: Points $(1, +1)$ and $(-1, -1)$ are the support vectors!

- These are closest to the decision boundary $x = 0$

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Answer: Points $(1, +1)$ and $(-1, -1)$ are the support vectors!

- These are closest to the decision boundary $x = 0$
- They satisfy $y_i(w \cdot x_i + b) = 1$ exactly

Pop Quiz #4

Support Vector Challenge!

In our 1D example with data points $\{(1,+1),(2,+1),(-1,-1),(-2,-1)\}$, which points will be the support vectors?

Think: Support vectors are the closest points to the decision boundary that actively constrain the solution.

Answer: Points $(1,+1)$ and $(-1,-1)$ are the support vectors!

- These are closest to the decision boundary $x = 0$
- They satisfy $y_i(w \cdot x_i + b) = 1$ exactly
- Points $(2,+1)$ and $(-2,-1)$ are farther away $\Rightarrow \alpha = 0$

Revisiting the Simple Example

$$
\begin{aligned}
L(\alpha_1, \alpha_2, \alpha_3, \alpha_4) = & \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 \\
& - \frac{1}{2} \{ \alpha_1 \alpha_1 \times (1 * 1) \times (1 * 1) \\
& \qquad + \\
& \alpha_1 \alpha_2 \times (1 * 1) \times (1 * 2) \\
& \qquad + \\
& \alpha_1 \alpha_3 \times (1 * -1) \times (1 * 1) \\
& \qquad \ldots \\
& \alpha_4 \alpha_4 \times (-1 * -1) \times (-2 * -2) \}
\end{aligned}
$$

How to Solve? $\Rightarrow$ Use the QP Solver!!

Revisiting the Simple Example

For the trivial example,

We know that only $x = \pm 1$ will take part in the constraint actively.

Thus, $\alpha_2, \alpha_4 = 0$

By symmetry, $\alpha_1 = \alpha_3 = \alpha$ (say)

& $\sum y_i \alpha_i = 0$

$$
\begin{aligned}
L(\alpha_1, \alpha_2, \alpha_3, \alpha_4) =& 2\alpha \\
& - \frac{1}{2} \{ \alpha^2 (1)(-1)(1)(-1) \\
& \quad + \alpha^2 (-1)(1)(-1)(1) \\
& \quad + \alpha^2 (1)(1)(1)(1) + \alpha^2 (-1)(-1)(-1)(-1) \\
& \}
\end{aligned}
$$

$$\underset{\alpha}{Maximize} \quad 2\alpha - \tfrac{1}{2}(4\alpha^2)$$

Revisiting the Simple Example

$$
\begin{aligned}
\frac{\partial}{\partial \alpha}\left(2\alpha - 2\alpha^2\right) &= 0 \Rightarrow 2 - 4\alpha = 0 \\
&\Rightarrow \;\alpha = 1/2 \\
\therefore \alpha_1 = 1/2 \;\; \alpha_2 = 0; \;\; \alpha_3 &= 1/2 \;\; \alpha_4 = 0 \\
\mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \bar{x}_i &= 1/2 \times 1 \times 1 + 0 \times 1 \times 2 \\
&\quad + 1/2 \times -1 \times -1 + 0 \times -1 \times -2 \\
&= 1/2 + 1/2 = 1
\end{aligned}
$$

Finding b:

For the support vectors we have,

$y_i(\mathbf{w} \cdot \mathbf{x}_i + b) - 1 = 0$

or, $y_i \ (\bar{w} \cdot \bar{x}_1 + b) = 1$

or, $y_i^2 \, (\bar{w} \cdot \bar{x}_i + b) = y_i$

or, $\quad \bar{w}, \bar{x}_i + b = y_i \ \ (\because y_i^2 = 1)$

or, $b = y_i - w \cdot x_i$

In practice, $b = \frac{1}{N_{SV}} \sum_{i=1}^{N_{SV}} (y_i - \bar{w}\bar{x}_i)$

Obtaining the Solution

$$
\begin{aligned}
b &= \frac{1}{2}\{(1-(1)(1)) + (-1-(1)(-1))\\
&= \frac{1}{2}\{0+0\} = 0\\
&= 0\\
&\therefore w = 1 \ \ \& \ \ b = 0
\end{aligned}
$$

Making Predictions

$$\hat{y}(x_i) = \text{SIGN}(w \cdot x_i + b)$$

For $x_{test} = 3$; $\hat{y}(3) = \text{SIGN}(1 \times 3 + 0) = +$ve class

Alternatively,

$$\begin{aligned}\hat{\mathbf{y}}(\mathbf{x}_{\text{test}}) &= \text{sign}(\mathbf{w} \cdot \mathbf{x}_{\text{test}} + b) \\ &= \text{sign}\left(\sum_{j=1}^{N_{\text{SV}}} \alpha_j y_j \mathbf{x}_j \cdot \mathbf{x}_{\text{test}} + b\right)\end{aligned}$$

In our example,

$\alpha_1 = 1/2; \alpha_2 = 0; \quad \alpha_3 = 1/2; \alpha_4 = 0$

$$\hat{\mathbf{y}}(3) = \text{sign}\left(\frac{1}{2} \times 1 \times (1 \times 3) + 0 + \frac{1}{2} \times (-1) \times (-1 \times 3) + 0\right)$$

$$= \text{sign}\left(\frac{6}{2}\right) = \text{sign}(3) = +1$$

Pop Quiz #5

Prediction Power!

We found our SVM solution: $w = 1, b = 0$. Let's test it!

What will our SVM predict for the test point $x_{\text{test}} = -0.5$?

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What will our SVM predict for the test point $x_{\text{test}} = -0.5$?

Method 1: Direct: $\hat{\mathbf{y}}(-0.5) = \text{sign}(1 \times (-0.5) + 0) = \text{sign}(-0.5) = -1$

Method 2: Using support vectors: $\hat{\mathbf{y}}(-0.5) = \text{sign}(\frac{1}{2} \times 1 \times 1 \times (-0.5) + \frac{1}{2} \times (-1) \times (-1) \times (-0.5)) = \text{sign}(-0.5) = -1$ (Correct!)

Kernel Methods

ORIGINAL DATA
IN R

Non-Linearly Separable Data

- Data is not linearly separable in $\mathbb{R}^d$.

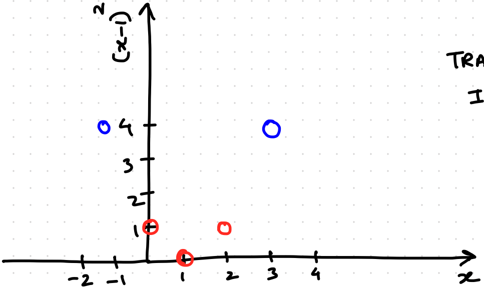
Non-Linearly Separable Data

- Data is not linearly separable in $\mathbb{R}^d$.
- Can we still use SVM?

Non-Linearly Separable Data

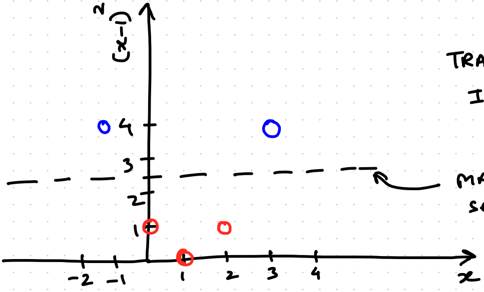
- Data is not linearly separable in $\mathbb{R}^d$.
- Can we still use SVM?
- Yes! Project data to a higher dimensional space.

ORIGINAL DATA
IN R



TRANSFORMED DATA
IN R^2

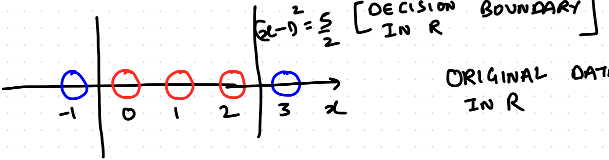
ORIGINAL DATA IN $\mathbb{R}$



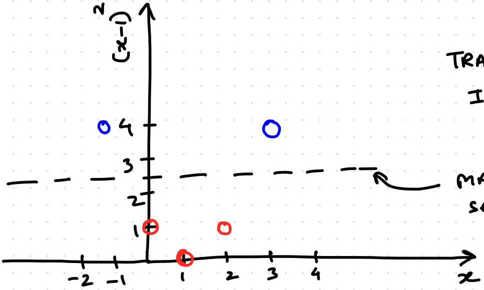
TRANSFORMED DATA IN $\mathbb{R}^2$

MAX MARGIN SEPARATING HYPERPLANE

$(x-1)^2 = \frac{5}{2}$



ORIGINAL DATA IN R



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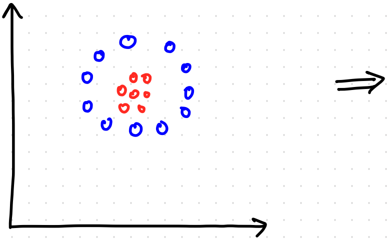
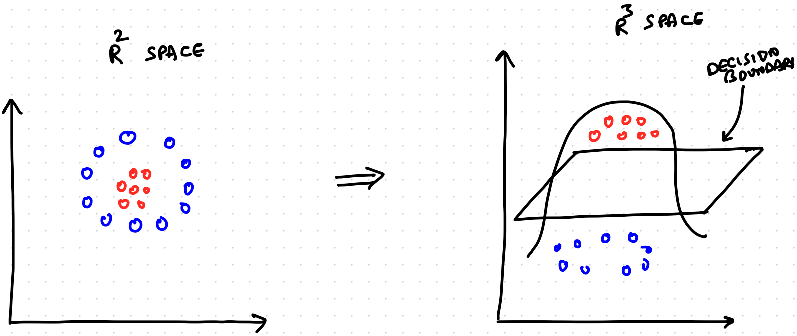
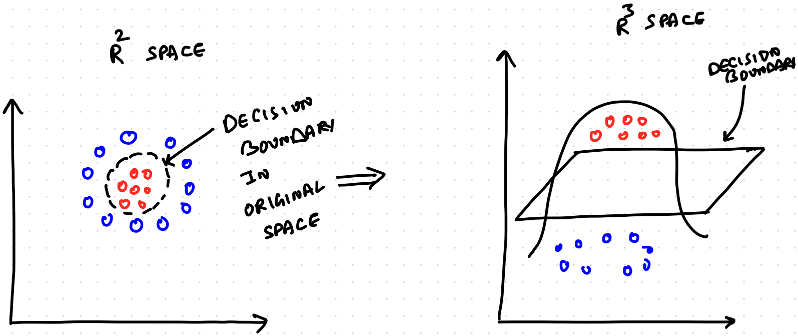
R^2 SPACE





R^2 SPACE
R^3 SPACE
DECISION BOUNDARY



R^2 SPACE
DECISION BOUNDARY IN ORIGINAL SPACE
R^3 SPACE
DECISION BOUNDARY

Projection/Transformation Function

$\phi : \mathbb{R}^d \rightarrow \mathbb{R}^D$

where, $d =$ original dimension

$D =$ new dimension

In our example:

$d = 1; D = 2$

From Linear to Kernel SVM

Linear SVM:

Maximize

$$L(\alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j$$

such that constriants are satisfied.

$$\downarrow$$

Transformation (ϕ)

$$\downarrow$$

$$L(\alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}_j)$$

Steps

1. Compute $\phi(\mathbf{x})$ for each point

$$\phi : \mathbb{R}^d \rightarrow \mathbb{R}^D$$

Q. If $D >> d$

Both steps are expensive!

Steps

1. Compute $\phi(\mathbf{x})$ for each point

$$\phi : \mathbb{R}^d \to \mathbb{R}^D$$

2. Compute dot products over $\mathbb{R}^D$ space

Q. If $D >> d$

Both steps are expensive!

Brilliant idea: Can we compute $K(\mathbf{x}_i, \mathbf{x}_j)$ such that:

$$K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}_j)$$

Without explicitly computing ϕ!

- $K(\mathbf{x}_i, \mathbf{x}_j)$: Simple function in original space

Result: Get non-linear classification power without computational cost!

The Kernel Trick

Brilliant idea: Can we compute $K(\mathbf{x}_i, \mathbf{x}_j)$ such that:

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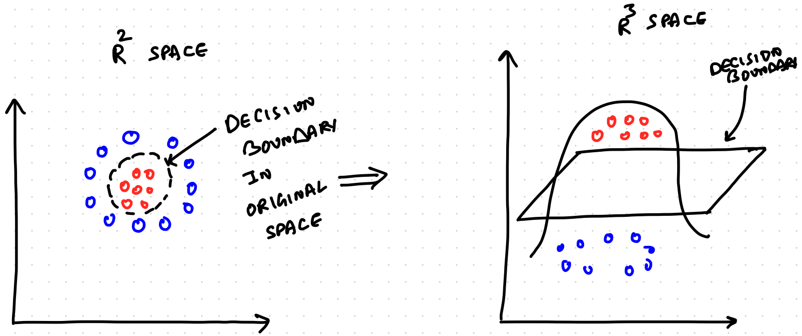
Without explicitly computing ϕ!

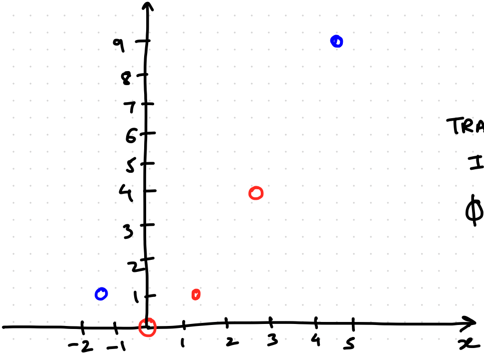
- $K(\mathbf{x}_i, \mathbf{x}_j)$: Simple function in original space
- $\phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}_j)$: Complex dot product in high-dimensional space

Result: Get non-linear classification power without computational cost!



R^2 SPACE
DECISION BOUNDARY IN ORIGINAL SPACE
R^3 SPACE
DECISION BOUNDARY

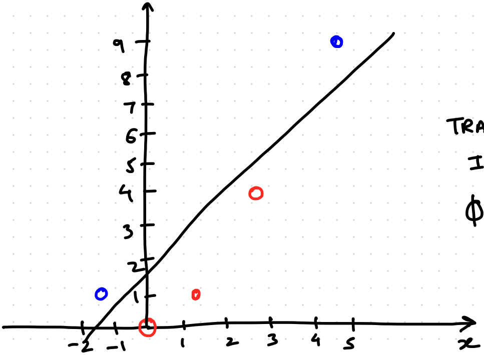
ORIGINAL DATA IN $\mathbb{R}$



TRANSFORMED DATA IN $\mathbb{R}^2$

$$\phi(x) = \begin{bmatrix} \sqrt{2}\,x \\ x^2 \end{bmatrix}$$

ORIGINAL DATA
IN $\mathbb{R}$



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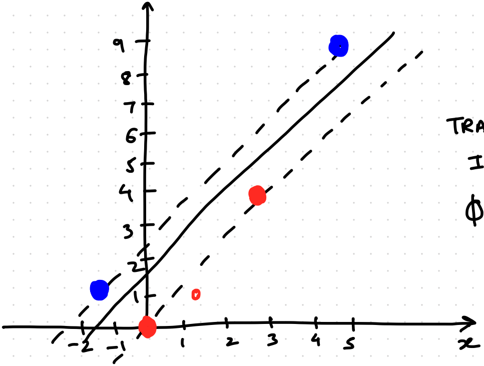

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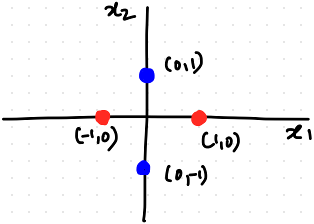
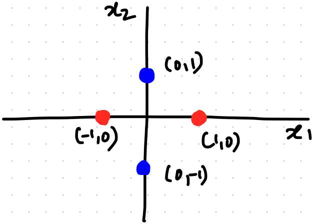


x_2
(0,1)
(-1,0)
(1,0)
x_1
(0,-1)



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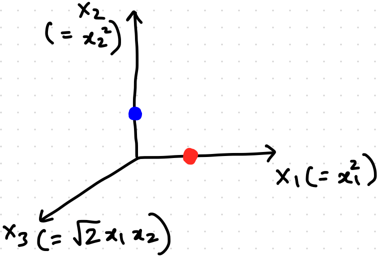
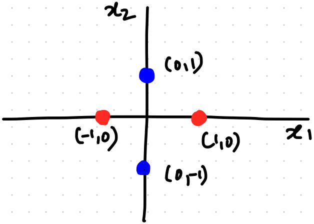


X_2
$(= x_2^2)$
$X_1 (= x_1^2)$
$X_3 (= \sqrt{2} x_1 x_2)$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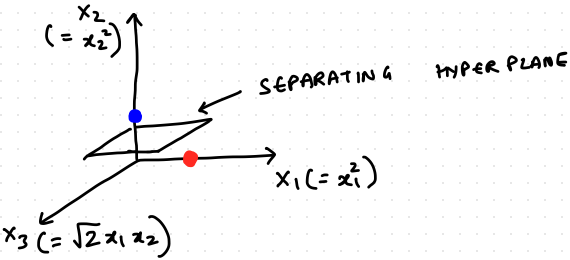
X_2 $(= x_2^2)$
SEPARATING HYPERPLANE
$X_1 (= x_1^2)$
$X_3 (= \sqrt{2} x_1 x_2)$

Kernel Trick

Q) Why did we use dual form?

Kernels again!!

Primal form doesn't allow for the kernel trick
$K(\mathbf{x}_1, \mathbf{x}_2)$ in dual and compute $\phi(\mathbf{x})$ and then dot product in D dimensions

Gram Matrix: (Positive Semi-Definite)

$K(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i \cdot \mathbf{x}_j)^2$

	x_1	x_2	x_3	x_4	x_5	x_6	x_7
x_1	24	8	0	0	8	24	48
x_2	8	1	0	-1	0	...	
x_3	0	...	...	...	...	...	...
x_4	0						
x_5	8						
x_6	24						
x_7	48						

Common Kernel Functions

Most frequently used kernels:

1. **Linear:** $K(\mathbf{x}_1, \mathbf{x}_2) = \mathbf{x}_1 \cdot \mathbf{x}_2$

Parameters:

Common Kernel Functions

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3. **RBF (Gaussian):** $K(\mathbf{x}_1, \mathbf{x}_2) = \exp(-\gamma \|\mathbf{x}_1 - \mathbf{x}_2\|^2)$

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Parameters:

- c: constant term, d: degree (polynomial)
- γ: bandwidth parameter (RBF)

Kernel Example: Polynomial Kernel

Question: For $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$, what is the feature space for $K(\mathbf{x}, \mathbf{z}) = (1 + \mathbf{x} \cdot \mathbf{z})^3$?

Given: $\mathbf{x} \in \mathbb{R}^2$, find dimension of $\phi(\mathbf{x})$

Expansion:

$$\begin{aligned} K(\mathbf{x}, \mathbf{z}) &= (1 + x_1 z_1 + x_2 z_2)^3 \\ &= \text{all terms of degree } \leq 3 \\ &= \phi(\mathbf{x}) \cdot \phi(\mathbf{z}) \end{aligned}$$

Feature map: $\phi(\mathbf{x}) = [1, \sqrt{3}x_1, \sqrt{3}x_2, \sqrt{3}x_1^2, \sqrt{3}x_2^2, \sqrt{6}x_1 x_2, x_1^3, x_2^3, \sqrt{3}x_1^2 x_2, \sqrt{3}x_1 x_2^2]$

Answer: $\phi(\mathbf{x}) \in \mathbb{R}^{10}$

RBF Kernel: Infinite Dimensions

Question: What is the dimensionality of RBF kernel feature space?

RBF Kernel:

$$\begin{aligned} K(x, z) &= \exp(-\gamma \|x - z\|^2) \\ &= \exp(-\gamma (x - z)^2) \end{aligned}$$

Key insight: Using Taylor series expansion

$$\exp(\alpha) = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} = 1 + \alpha + \frac{\alpha^2}{2!} + \frac{\alpha^3}{3!} + \cdots$$

Result: RBF kernel corresponds to ∞-dimensional feature space!

Amazing: Infinite-dimensional classification with finite computation!

Does RBF Involve Dot Product in Lower-Dimensional Space?

Question: Can we see the original dot product in RBF kernel?

Assuming **x** is a one-dimensional vector, we can rewrite the RBF kernel as:

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Expanding the squared term:

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Substituting back into the RBF kernel:

$$\begin{aligned} K(x, z) &= \exp(-\gamma (x^2 - 2xz + z^2)) \\ &= \exp(-\gamma x^2) \cdot \exp(2\gamma xz) \cdot \exp(-\gamma z^2) \end{aligned}$$

Key insight: The middle term $\exp(2\gamma xz)$ contains the dot product xz from the original space!

SVM: Parametric vs Non-Parametric

Question: Is SVM parametric or non-parametric?

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  - Fixed functional form
  - Number of parameters independent of training data size
- **Non-parametric:** RBF kernel
  - Model complexity grows with data

SVM: Parametric vs Non-Parametric

Question: Is SVM parametric or non-parametric?

Answer: It depends on the kernel!

- **Parametric:** Linear and polynomial kernels
  - Fixed functional form
  - Number of parameters independent of training data size
- **Non-parametric:** RBF kernel
  - Model complexity grows with data
  - Uses all support vectors for prediction

RBF is Non-Parametric

$$
\begin{aligned}
\hat{\mathbf{y}}(\mathbf{x}_{\text{test}}) &= \text{sign}(\mathbf{w} \cdot \mathbf{x}_{\text{test}} + b) \\
&= \text{sign}(\sum_{j=1}^{N_{\text{SV}}} \alpha_j y_j \mathbf{x}_j \cdot \mathbf{x}_{\text{test}} + b) \\
\hat{\mathbf{y}}(\mathbf{x}_{\text{test}}) &= \text{sign}(\sum_{j=1}^{N} \alpha_j y_j K(\mathbf{x}_j, \mathbf{x}_{\text{test}}) + b)
\end{aligned}
$$

$\alpha_j = 0$ where $j \neq$ S.V.

Interpretation of RBF

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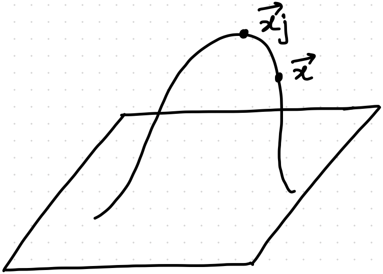
- $\exp(-\|\mathbf{x} - \mathbf{x}_i\|^2)$ is the basis component

RBF INTERPRETATION



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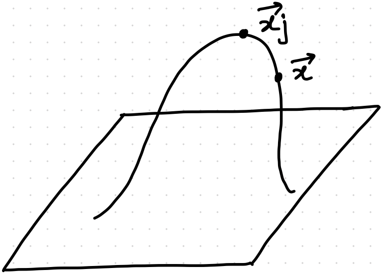
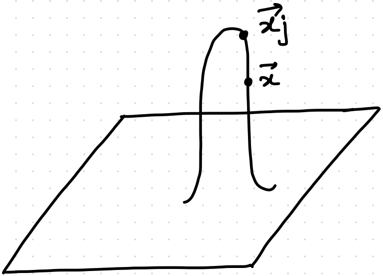


LOW γ

HIGH INFLUENCE OF $\vec{x}_j$



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Summary

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- **Flexibility:** Parametric (linear/poly) or non-parametric (RBF)
- **Efficiency:** Only support vectors matter for prediction

Next Steps

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